Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

pH-metric Result

logP (XH +)   0.59   ±0.04 (n=50)
logP (neutral X)   4.03   ±0.01 (n=50)

18C-03012 Points 1 to 26

M02_octanol concentration factor   0.955
Carbonate   0.2235 mM
Acidity error   -1.42826 mM

18C-03012 Points 27 to 50

M02_octanol concentration factor   0.892
Carbonate   0.1033 mM
Acidity error   -1.59633 mM

18C-03012 Points 51 to 75

M02_octanol concentration factor   1.218
Carbonate   0.1516 mM
Acidity error   -1.31894 mM
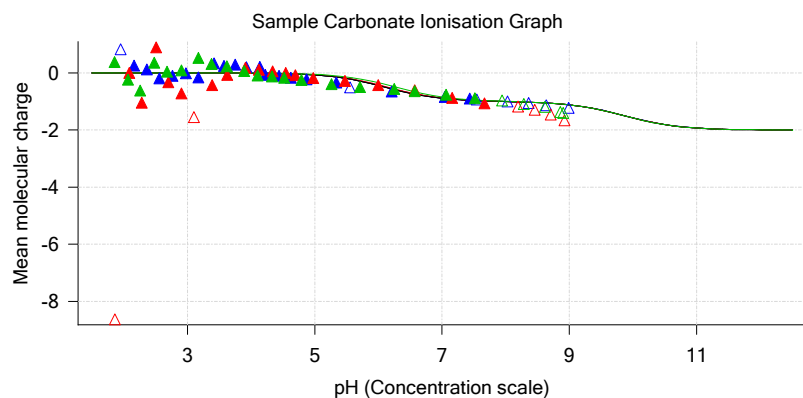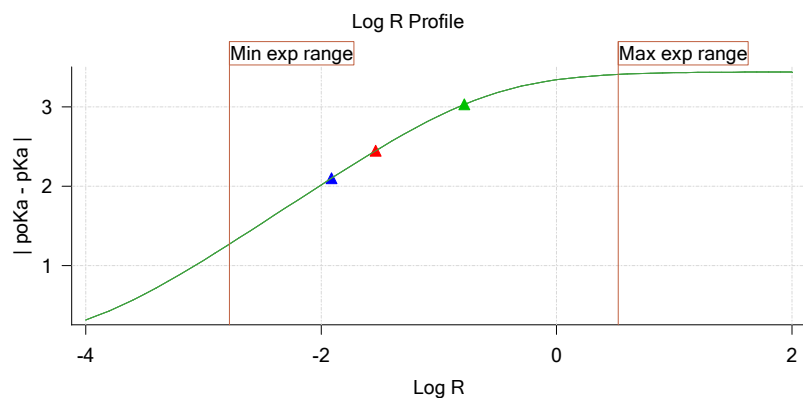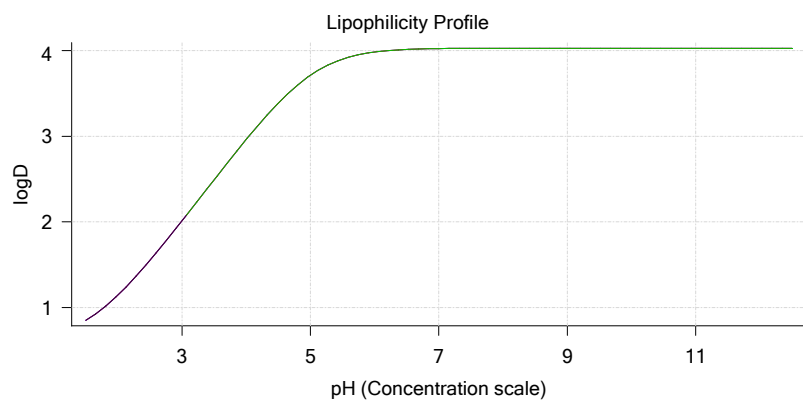
Warnings and errors
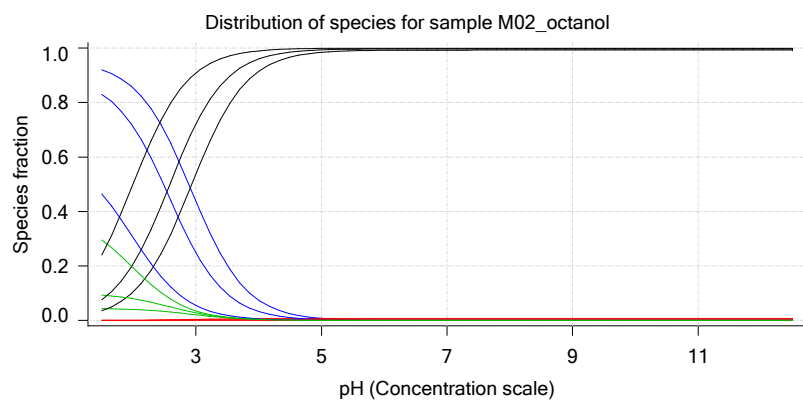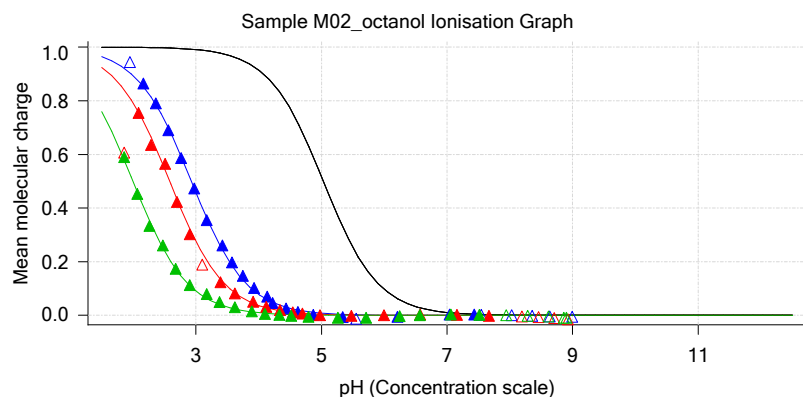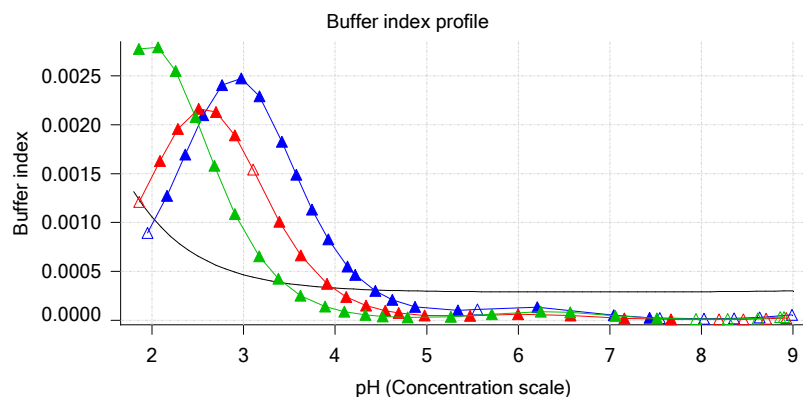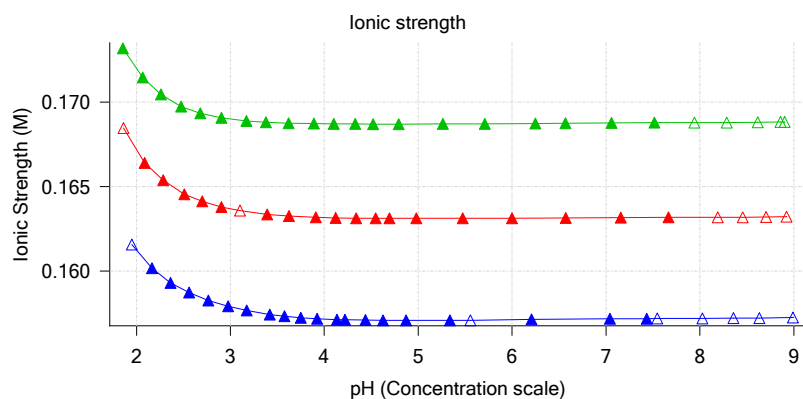
Errors   None
Warnings   None

Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanol	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	0.69	17.03 %	0.00 %	65.96 %	17.01 %	
1.200	0.74	15.49 %	0.00 %	59.99 %	24.51 %	Stomach pH
2.000	1.14	6.73 %	0.01 %	26.06 %	67.20 %	
3.000	2.01	0.95 %	0.01 %	3.70 %	95.34 %	
4.000	2.96	0.10 %	0.01 %	0.39 %	99.51 %	
5.000	3.71	0.01 %	0.01 %	0.04 %	99.94 %	
6.000	3.99	0.00 %	0.01 %	0.00 %	99.99 %	
6.500	4.01	0.00 %	0.01 %	0.00 %	99.99 %	
7.000	4.02	0.00 %	0.01 %	0.00 %	99.99 %	
7.400	4.03	0.00 %	0.01 %	0.00 %	99.99 %	Blood pH
8.000	4.03	0.00 %	0.01 %	0.00 %	99.99 %	
9.000	4.03	0.00 %	0.01 %	0.00 %	99.99 %	
10.000	4.03	0.00 %	0.01 %	0.00 %	99.99 %	
11.000	4.03	0.00 %	0.01 %	0.00 %	99.99 %	
12.000	4.03	0.00 %	0.01 %	0.00 %	99.99 %	

pH-metric Result

Sample name: **M02_octanol** Experiment start time: **3/3/2018 3:08:32 PM**
Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
Assay ID: **18C-03012** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Graphs

Charge balance residuals

Ionic strength

Buffer index profile

Sample M02_octanol Ionisation Graph

Distribution of species for sample M02_octanol

Lipophilicity Profile

Log R Profile

Sample Carbonate Ionisation Graph

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
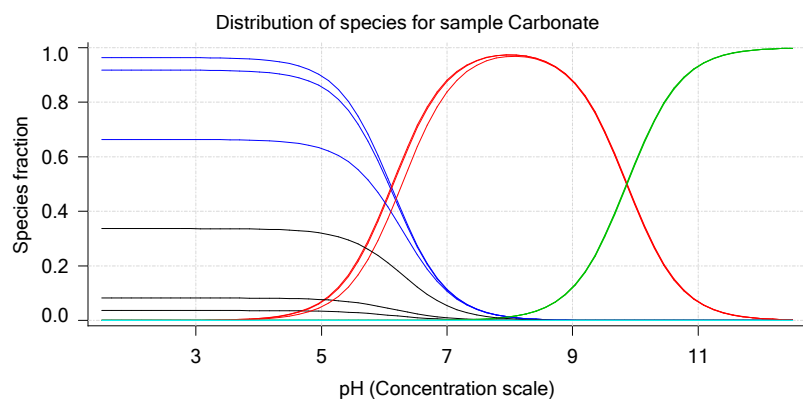Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Graphs (continued)

Distribution of species for sample Carbonate

Sample name: **M02_octanol**   Experiment start time: **3/3/2018 3:08:32 PM**
Assay name: **pH-metric high logP**   Analyst: **Dorothy Levorse**
Assay ID: **18C-03012**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

pH-metric high logP   Titration 1 of 3   18C-03012 Points 1 to 26

Overall results

RMSD   0.169
Average ionic strength   0.158 M
Average temperature   24.9°C
Partition ratio   0.0123 : 1
Analyte concentration range   4430.5 µM to 4567.1 µM
Total points considered   19 of 26

Warnings and errors

Errors   None
Warnings   Excessive acidity error present

Four-Plus parameters

🔒	Alpha	0.111	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	S	0.9988	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	jH	1.0	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	jOH	-0.8	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r

Titrants

🔒	0.50 M HCl	0.999058	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	0.50 M KOH	0.999845	3/3/2018 3:08:32 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

🔻	M02_octanol concentration factor	0.955
🔒	Base pKa 1	5.03
🔻	logP (XH +)	1.12
🔻	logP (neutral X)	4.07

Sample graphs

Ionisation of sample M02_octanol

Distribution of species for sample M02_octanol

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile
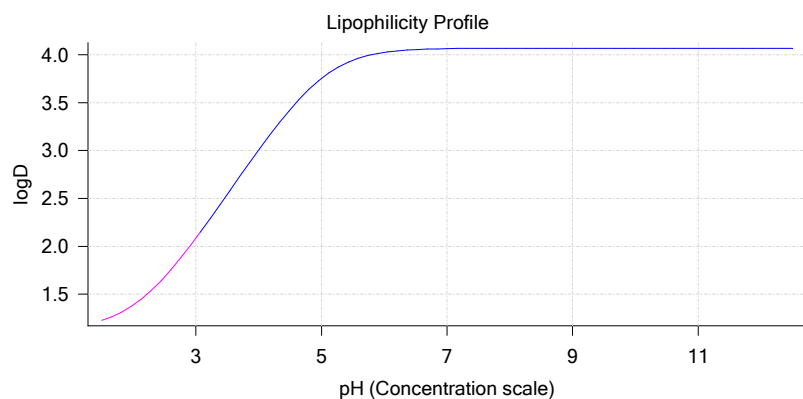
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanol	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	1.16	84.96 %	0.01 %	13.89 %	1.14 %	
1.200	1.18	84.39 %	0.01 %	13.80 %	1.79 %	Stomach pH
2.000	1.38	77.00 %	0.07 %	12.59 %	10.33 %	
3.000	2.08	39.77 %	0.37 %	6.50 %	53.36 %	
4.000	3.01	6.81 %	0.64 %	1.11 %	91.44 %	
5.000	3.75	0.73 %	0.68 %	0.12 %	98.46 %	
6.000	4.02	0.07 %	0.69 %	0.01 %	99.22 %	
6.500	4.05	0.02 %	0.69 %	0.00 %	99.28 %	
7.000	4.06	0.01 %	0.69 %	0.00 %	99.30 %	
7.400	4.07	0.00 %	0.69 %	0.00 %	99.31 %	Blood pH
8.000	4.07	0.00 %	0.69 %	0.00 %	99.31 %	
9.000	4.07	0.00 %	0.69 %	0.00 %	99.31 %	
10.000	4.07	0.00 %	0.69 %	0.00 %	99.31 %	
11.000	4.07	0.00 %	0.69 %	0.00 %	99.31 %	
12.000	4.07	0.00 %	0.69 %	0.00 %	99.31 %	

Carbonate and acidity

Carbonate 0.223 mM
Acidity error -1.428 mM

Other graphs

Assay progress

Titration graph

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
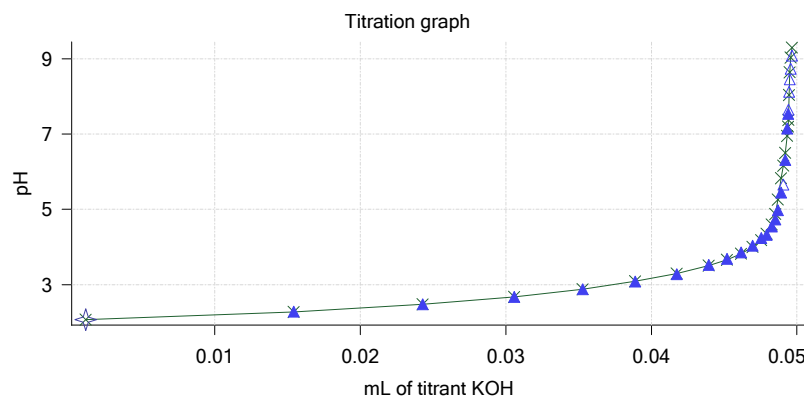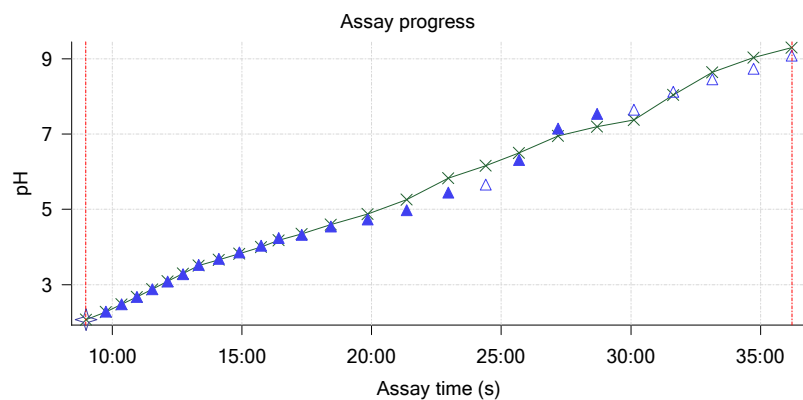Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
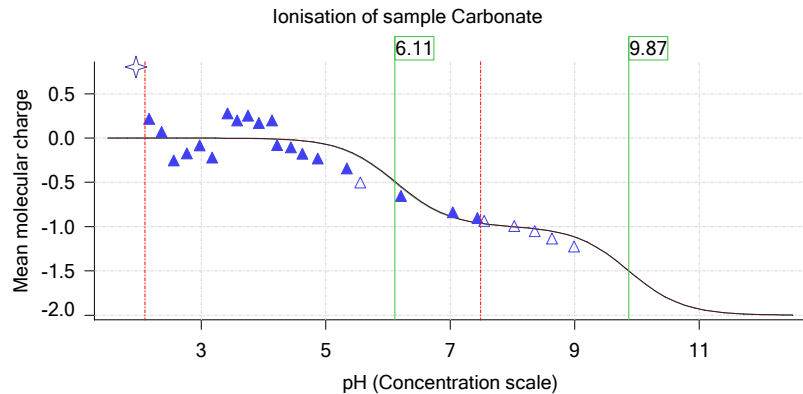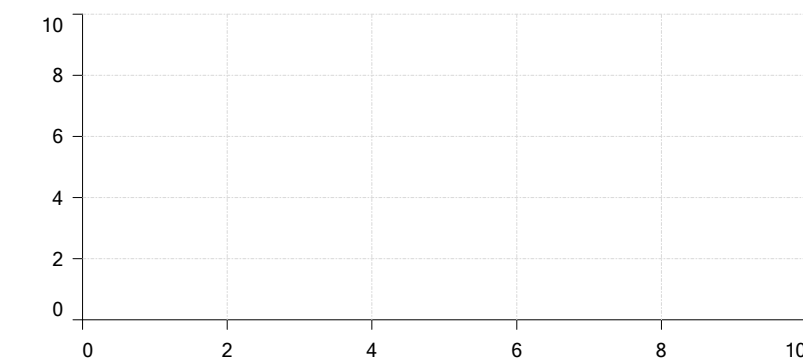
Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

pH-metric high logP   Titration 2 of 3   18C-03012 Points 27 to 50

Overall results

RMSD   0.235
Average ionic strength   0.163 M
Average temperature   25.0°C
Partition ratio   0.0290 : 1
Analyte concentration range   4080.4 µM to 4209.4 µM
Total points considered   18 of 24

Warnings and errors

Errors   None
Warnings   Excessive acidity error present

Four-Plus parameters

🔒	Alpha	0.111	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	S	0.9988	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	jH	1.0	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	jOH	-0.8	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r

Titrants

🔒	0.50 M HCl	0.999058	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r
🔒	0.50 M KOH	0.999845	3/3/2018 3:08:32 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

🔻	M02_octanol concentration factor	0.892
🔒	Base pKa 1	5.03
🔻	logP (XH +)	1.47
🔻	logP (neutral X)	4.27

Sample graphs

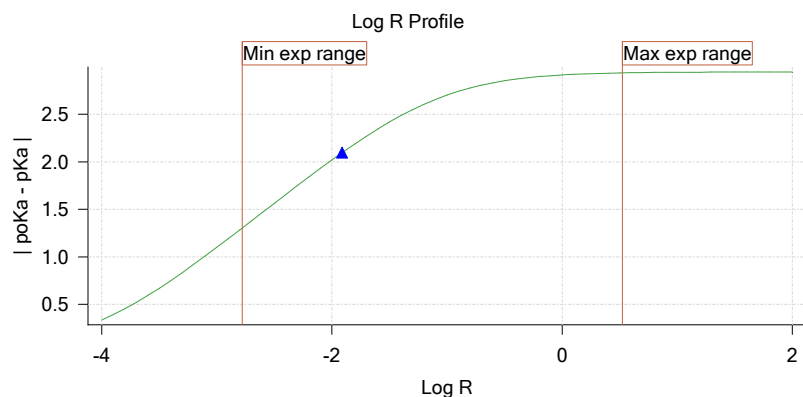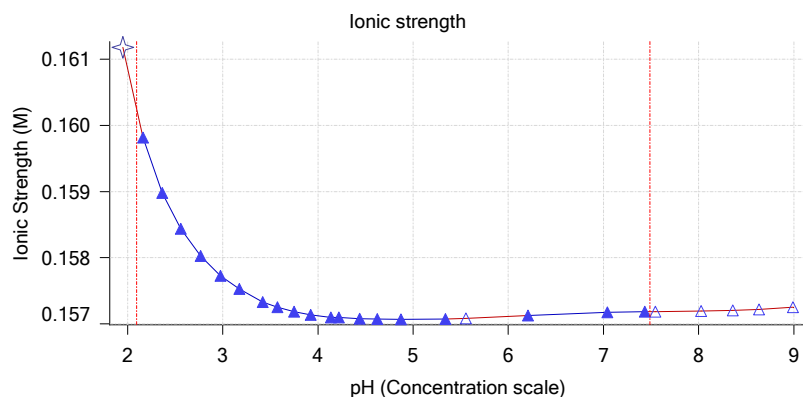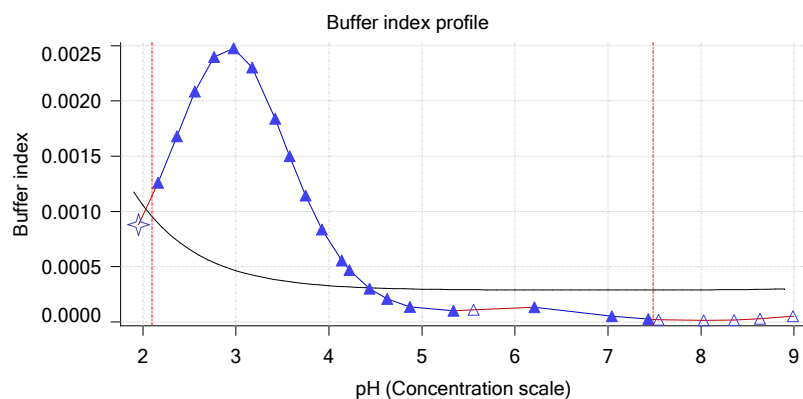Ionisation of sample M02_octanol

Distribution of species for sample M02_octanol
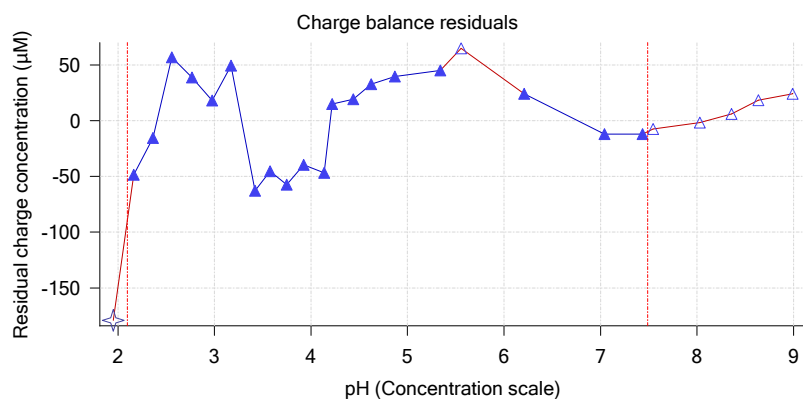
Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile
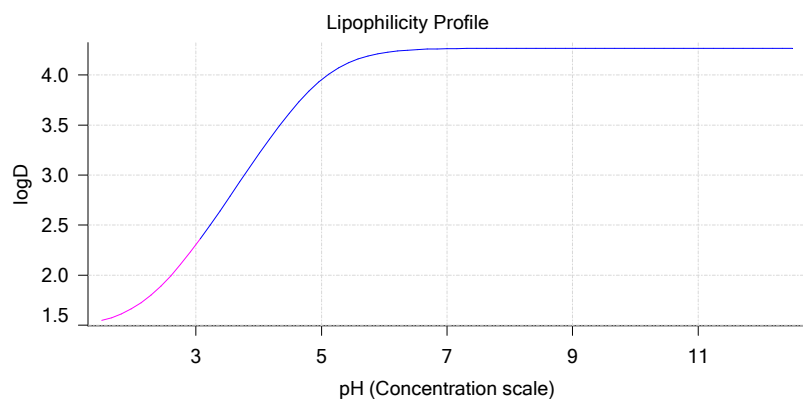
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanol	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	1.50	52.20 %	0.00 %	45.17 %	2.62 %	
1.200	1.51	51.41 %	0.01 %	44.49 %	4.09 %	Stomach pH
2.000	1.67	42.22 %	0.04 %	36.54 %	21.21 %	
3.000	2.30	14.50 %	0.14 %	12.55 %	72.82 %	
4.000	3.21	1.92 %	0.18 %	1.66 %	96.25 %	
5.000	3.95	0.20 %	0.18 %	0.17 %	99.45 %	
6.000	4.22	0.02 %	0.19 %	0.02 %	99.78 %	
6.500	4.25	0.01 %	0.19 %	0.01 %	99.80 %	
7.000	4.26	0.00 %	0.19 %	0.00 %	99.81 %	
7.400	4.27	0.00 %	0.19 %	0.00 %	99.81 %	Blood pH
8.000	4.27	0.00 %	0.19 %	0.00 %	99.81 %	
9.000	4.27	0.00 %	0.19 %	0.00 %	99.81 %	
10.000	4.27	0.00 %	0.19 %	0.00 %	99.81 %	
11.000	4.27	0.00 %	0.19 %	0.00 %	99.81 %	
12.000	4.27	0.00 %	0.19 %	0.00 %	99.81 %	

Carbonate and acidity

Carbonate   0.103 mM
Acidity error   -1.596 mM

Other graphs

Assay progress

Titration graph

Sample name: **M02_octanol** Experiment start time: **3/3/2018 3:08:32 PM**
Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
Assay ID: **18C-03012** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

pH-metric high logP   Titration 3 of 3   18C-03012 Points 51 to 75

Overall results

RMSD   0.321
Average ionic strength   0.169 M
Average temperature   25.0°C
Partition ratio   0.1643 : 1
Analyte concentration range   3372.3 µM to 3470.6 µM
Total points considered   20 of 25

Warnings and errors

Errors   None
Warnings   Excessive acidity error present

Four-Plus parameters

	Alpha	0.111	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r
	S	0.9988	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r
	jH	1.0	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r
	jOH	-0.8	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r

Titrants

	0.50 M HCl	0.999058	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r
	0.50 M KOH	0.999845	3/3/2018 3:08:32 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

	M02_octanol concentration factor	1.218
	Base pKa 1	5.03
	logP (XH +)	1.33
	logP (neutral X)	4.47

Sample graphs

Ionisation of sample M02_octanol

Distribution of species for sample M02_octanol

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
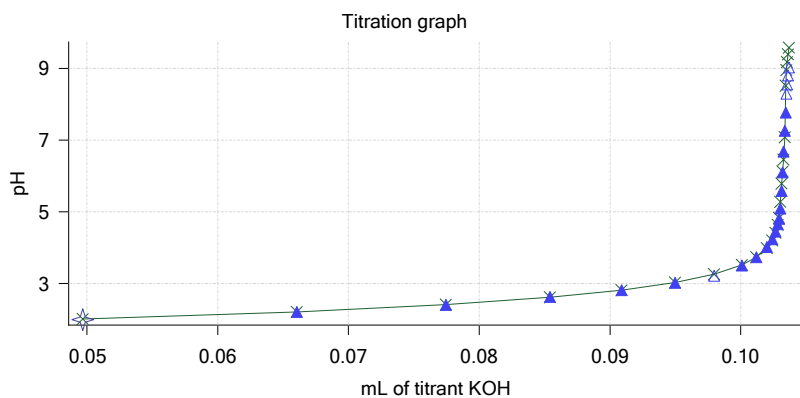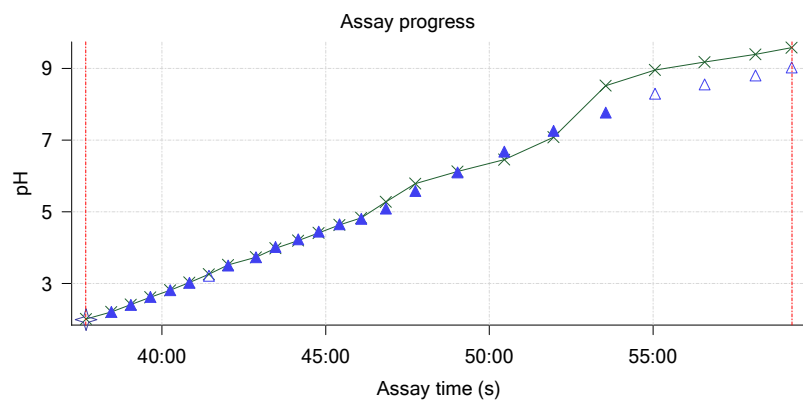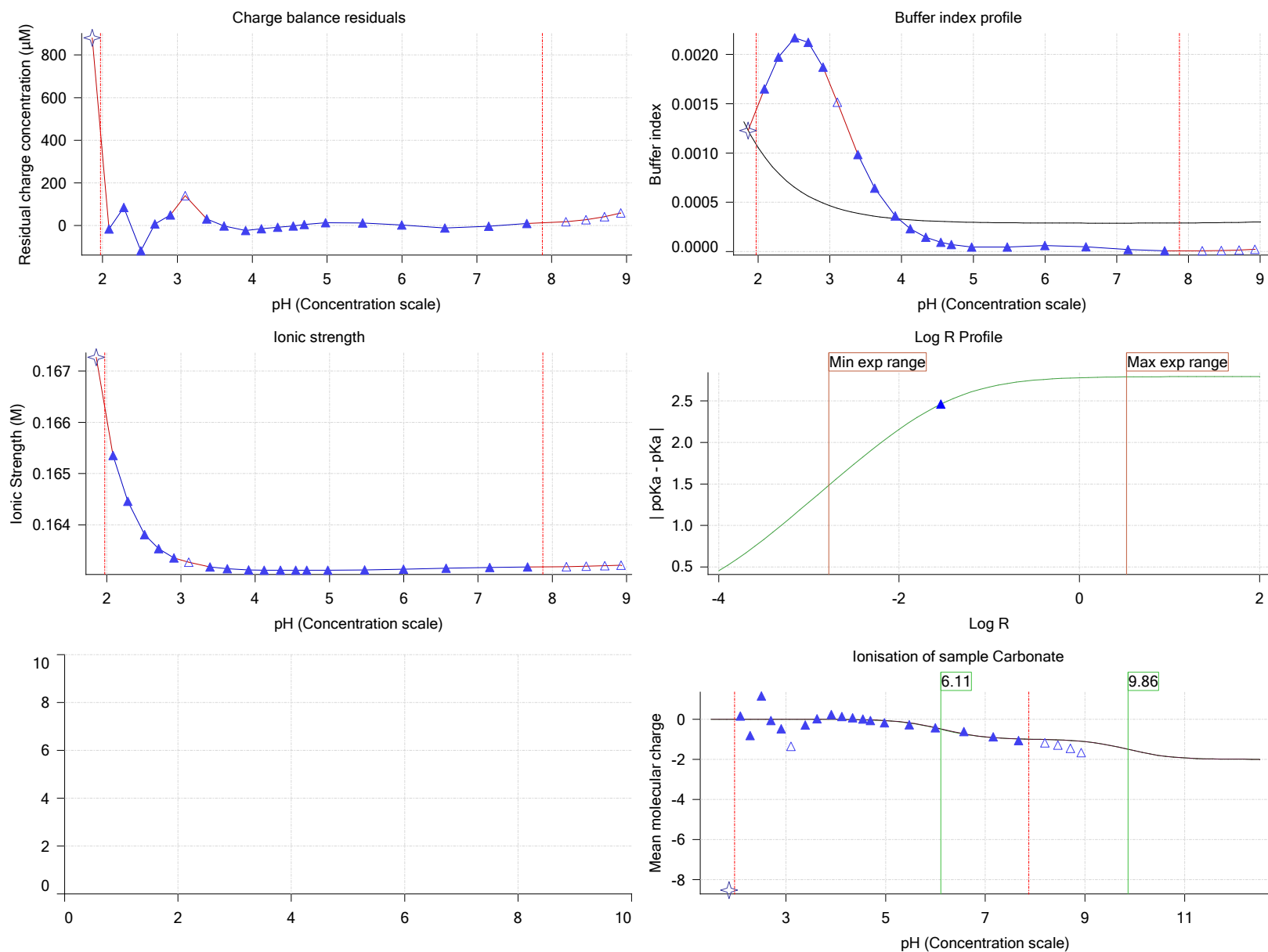Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile
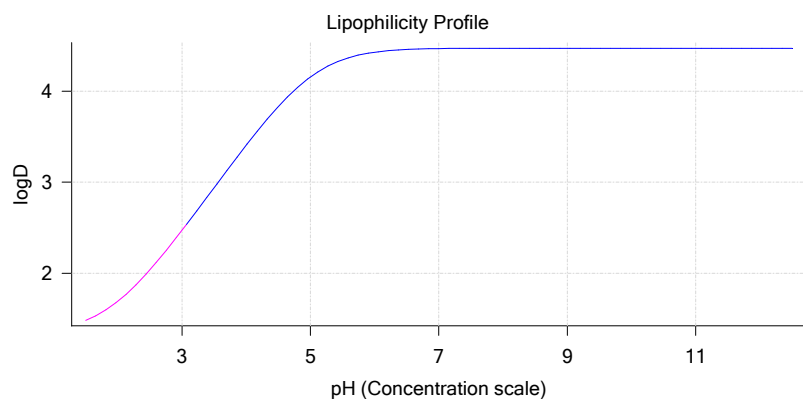
Sample logD and percent species

pH	M02_octanol logD	M02_octanol M02_octanolH	M02_octanol M02_octanol	M02_octanol M02_octanolH*	M02_octanol M02_octanol*	Comment
1.000	1.39	20.05 %	0.00 %	70.82 %	9.14 %	
1.200	1.41	19.03 %	0.00 %	67.22 %	13.74 %	Stomach pH
2.000	1.69	11.00 %	0.01 %	38.86 %	50.13 %	
3.000	2.47	2.00 %	0.02 %	7.05 %	90.94 %	
4.000	3.41	0.22 %	0.02 %	0.77 %	99.00 %	
5.000	4.16	0.02 %	0.02 %	0.08 %	99.88 %	
6.000	4.43	0.00 %	0.02 %	0.01 %	99.97 %	
6.500	4.46	0.00 %	0.02 %	0.00 %	99.98 %	
7.000	4.47	0.00 %	0.02 %	0.00 %	99.98 %	
7.400	4.47	0.00 %	0.02 %	0.00 %	99.98 %	Blood pH
8.000	4.47	0.00 %	0.02 %	0.00 %	99.98 %	
9.000	4.47	0.00 %	0.02 %	0.00 %	99.98 %	
10.000	4.47	0.00 %	0.02 %	0.00 %	99.98 %	
11.000	4.47	0.00 %	0.02 %	0.00 %	99.98 %	
12.000	4.47	0.00 %	0.02 %	0.00 %	99.98 %	

Carbonate and acidity

Carbonate   0.152 mM
Acidity error   -1.319 mM

Other graphs

Assay progress

Titration graph

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile
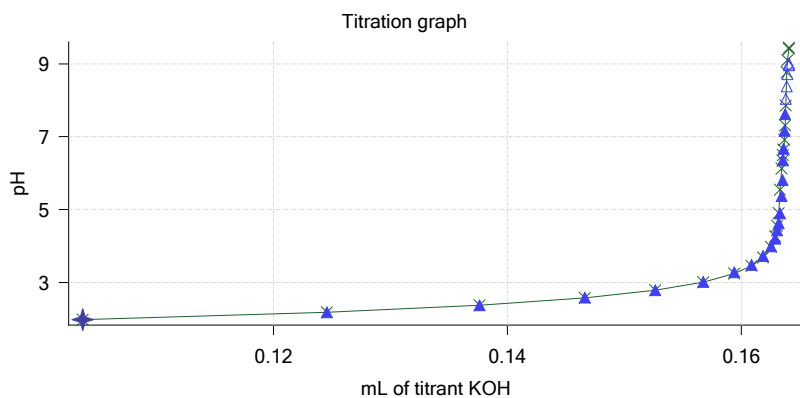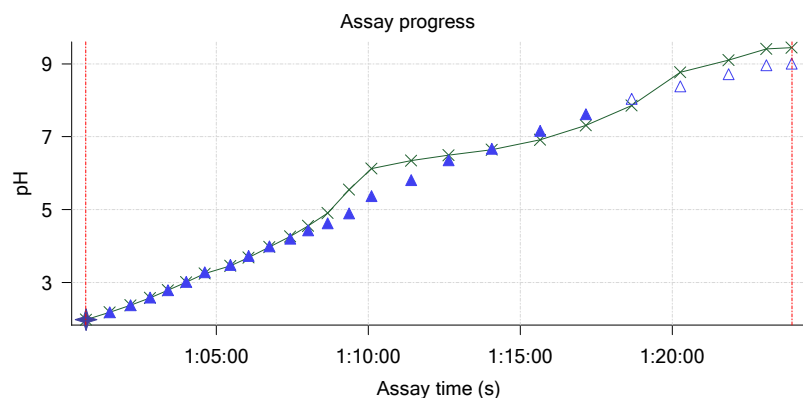

Ionisation of sample Carbonate
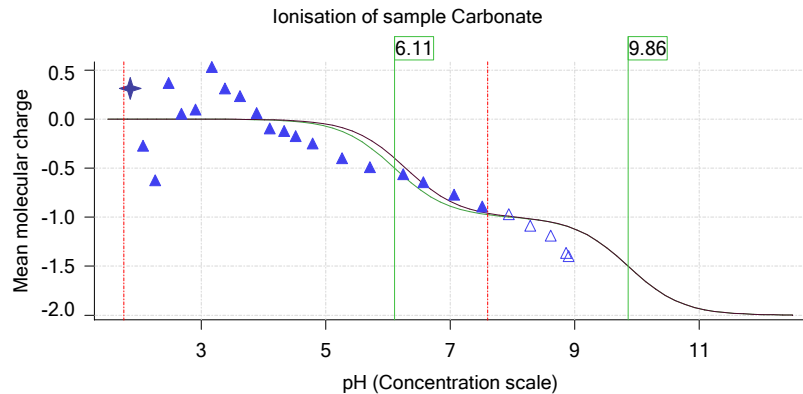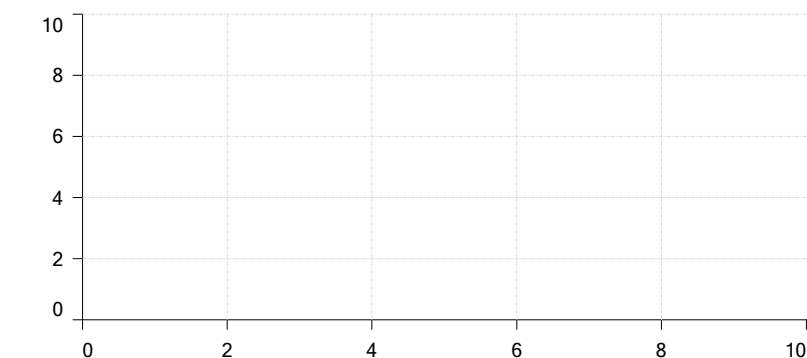
Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M02_octanol	12/6/2017 4:20:03 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.002080 g	3/2/2018 5:10:06 PM	User entered value
Formula weight	289.26 g/mol	12/6/2017 4:20:03 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	289.26	12/6/2017 4:20:03 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	12/6/2017 4:20:03 PM	User entered value
Sample is a	Base	12/6/2017 4:20:03 PM	User entered value
pKa 1	5.03	12/6/2017 4:20:03 PM	User entered value
logp (XH +)	1.32	3/2/2018 3:38:13 PM	User entered value
logP (neutral X)	4.10	3/2/2018 3:38:07 PM	User entered value

Events

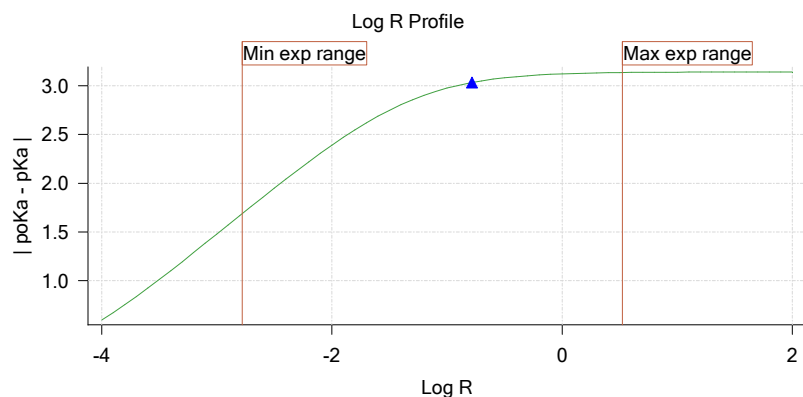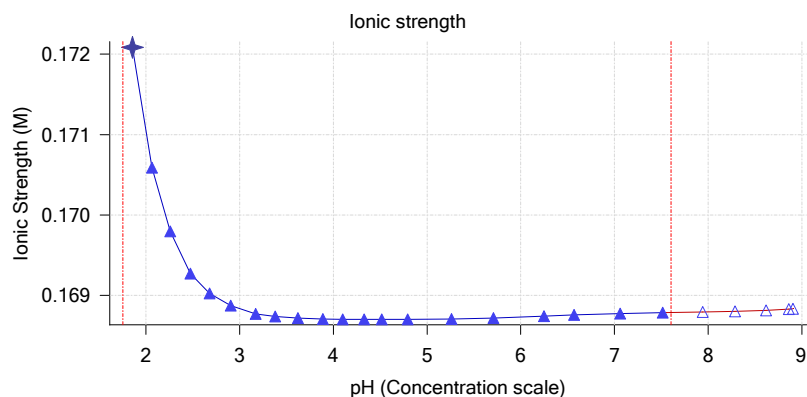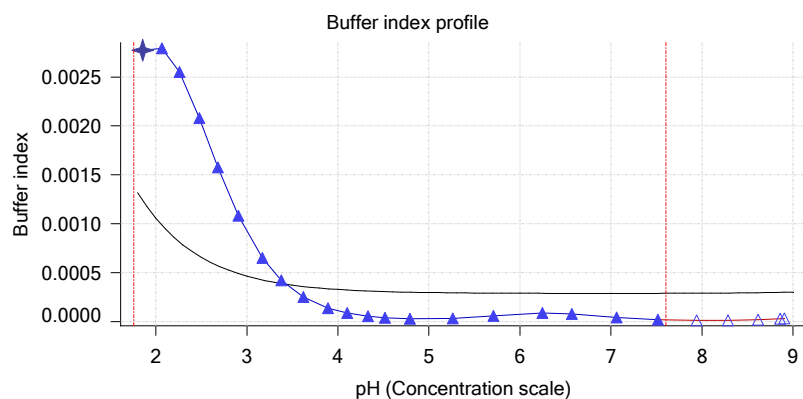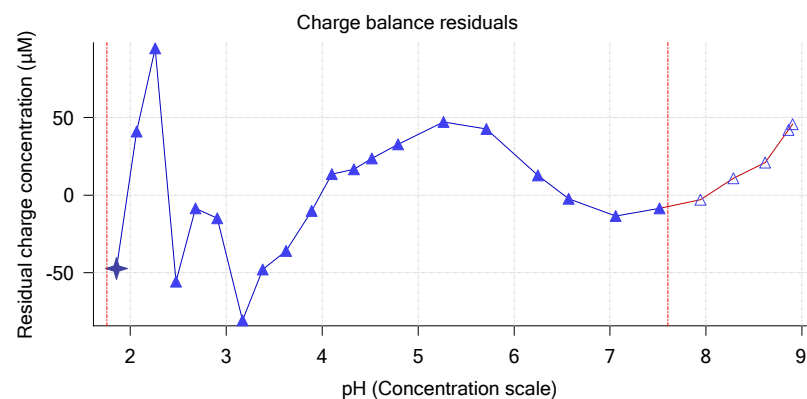| Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
5:59.7	Initial pH = 9.32									
8:59.2	Data point 1	1.50000 mL	0.05336 mL	0.00113 mL	0.01999 mL	2.071	0.00065	0.01575	0.00025	10.0 s
9:45.5	Data point 2	1.50000 mL	0.05336 mL	0.01543 mL	0.01999 mL	2.279	0.00438	0.13165	0.00060	10.0 s
10:21.2	Data point 3	1.50000 mL	0.05336 mL	0.02429 mL	0.01999 mL	2.476	-0.00354	0.41455	0.00027	10.5 s
10:57.3	Data point 4	1.50000 mL	0.05336 mL	0.03057 mL	0.01999 mL	2.669	-0.00471	0.73726	0.00027	10.0 s
11:32.8	Data point 5	1.50000 mL	0.05336 mL	0.03528 mL	0.01999 mL	2.875	-0.00270	0.03691	0.00069	10.0 s
12:08.2	Data point 6	1.50000 mL	0.05336 mL	0.03890 mL	0.01999 mL	3.083	-0.01251	0.86143	0.00067	10.0 s
12:43.7	Data point 7	1.50000 mL	0.05336 mL	0.04175 mL	0.01999 mL	3.280	-0.01215	0.94698	0.00062	10.5 s
13:19.6	Data point 8	1.50000 mL	0.05336 mL	0.04396 mL	0.01999 mL	3.527	-0.01947	0.93803	0.00099	11.0 s
14:06.4	Data point 9	1.50000 mL	0.05336 mL	0.04520 mL	0.01999 mL	3.683	-0.01786	0.92590	0.00092	11.5 s
14:53.7	Data point 10	1.50000 mL	0.05336 mL	0.04617 mL	0.01999 mL	3.855	-0.01936	0.96090	0.00098	14.5 s
15:44.0	Data point 11	1.50000 mL	0.05336 mL	0.04697 mL	0.01999 mL	4.031	-0.01779	0.90907	0.00092	15.5 s
16:24.9	Data point 12	1.50000 mL	0.05336 mL	0.04755 mL	0.01999 mL	4.242	-0.01825	0.89567	0.00095	28.0 s
17:18.3	Data point 13	1.50000 mL	0.05336 mL	0.04793 mL	0.01999 mL	4.326	-0.01954	0.97542	0.00098	36.5 s
18:25.4	Data point 14	1.50000 mL	0.05336 mL	0.04828 mL	0.01999 mL	4.543	-0.01825	0.97150	0.00091	55.0 s
19:50.9	Data point 15	1.50000 mL	0.05336 mL	0.04852 mL	0.01999 mL	4.730	-0.02010	0.91878	0.00103	Timed out at 59.5 s
21:21.5	Data point 16	1.50000 mL	0.05336 mL	0.04871 mL	0.01999 mL	4.975	-0.02384	0.95065	0.00121	Timed out at 59.5 s
22:57.2	Data point 17	1.50000 mL	0.05336 mL	0.04892 mL	0.01999 mL	5.443	-0.01935	0.93030	0.00099	56.0 s
24:23.8	Data point 18	1.50000 mL	0.05336 mL	0.04906 mL	0.01999 mL	5.658	-0.01989	0.98952	0.00099	46.5 s
25:40.9	Data point 19	1.50000 mL	0.05336 mL	0.04920 mL	0.01999 mL	6.311	-0.02340	0.95639	0.00118	Timed out at 59.5 s
27:11.5	Data point 20	1.50000 mL	0.05336 mL	0.04934 mL	0.01999 mL	7.143	-0.06220	0.99094	0.00309	Timed out at 59.5 s
28:41.9	Data point 21	1.50000 mL	0.05336 mL	0.04939 mL	0.01999 mL	7.536	-0.06100	0.98752	0.00303	Timed out at 59.5 s
30:07.3	Data point 22	1.50000 mL	0.05336 mL	0.04941 mL	0.01999 mL	7.646	-0.04673	0.98883	0.00232	Timed out at 59.5 s
31:37.8	Data point 23	1.50000 mL	0.05336 mL	0.04946 mL	0.01999 mL	8.129	-0.05480	0.98555	0.00273	Timed out at 59.5 s
33:08.3	Data point 24	1.50000 mL	0.05336 mL	0.04951 mL	0.01999 mL	8.458	-0.03117	0.96668	0.00157	Timed out at 59.5 s
34:43.9	Data point 25	1.50000 mL	0.05336 mL	0.04958 mL	0.01999 mL	8.734	-0.01915	0.91772	0.00099	57.5 s
36:12.1	Data point 26	1.50000 mL	0.05336 mL	0.04967 mL	0.01999 mL	9.090	-0.01873	0.92804	0.00096	35.5 s
37:41.3	Data point 27	1.50000 mL	0.10861 mL	0.04967 mL	0.05000 mL	1.983	-0.00848	0.30185	0.00076	10.0 s
38:27.6	Data point 28	1.50000 mL	0.10861 mL	0.06604 mL	0.05000 mL	2.203	-0.01236	0.74273	0.00071	10.0 s
39:03.3	Data point 29	1.50000 mL	0.10861 mL	0.07745 mL	0.05000 mL	2.397	-0.00234	0.07442	0.00042	10.0 s
39:38.9	Data point 30	1.50000 mL	0.10861 mL	0.08540 mL	0.05000 mL	2.621	-0.00166	0.44144	0.00012	10.5 s
40:15.0	Data point 31	1.50000 mL	0.10861 mL	0.09087 mL	0.05000 mL	2.809	-0.00504	0.92869	0.00026	10.0 s
40:50.5	Data point 32	1.50000 mL	0.10861 mL	0.09497 mL	0.05000 mL	3.014	-0.00539	0.66005	0.00033	10.0 s

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
41:26.0	Data point 33	1.50000 mL	0.10861 mL	0.09795 mL	0.05000 mL	3.211	-0.00572	0.74071	0.00033	10.0 s
42:01.6	Data point 34	1.50000 mL	0.10861 mL	0.10009 mL	0.05000 mL	3.497	-0.01360	0.48807	0.00096	10.0 s
42:52.5	Data point 35	1.50000 mL	0.10861 mL	0.10120 mL	0.05000 mL	3.730	0.00574	0.19061	0.00065	10.5 s
43:28.4	Data point 36	1.50000 mL	0.10861 mL	0.10200 mL	0.05000 mL	4.017	-0.01503	0.86567	0.00080	11.0 s
44:09.9	Data point 37	1.50000 mL	0.10861 mL	0.10240 mL	0.05000 mL	4.227	-0.01947	0.92718	0.00100	12.0 s
44:47.3	Data point 38	1.50000 mL	0.10861 mL	0.10266 mL	0.05000 mL	4.444	-0.01821	0.92624	0.00093	13.0 s
45:25.7	Data point 39	1.50000 mL	0.10861 mL	0.10282 mL	0.05000 mL	4.652	-0.01914	0.89982	0.00100	14.0 s
46:05.1	Data point 40	1.50000 mL	0.10861 mL	0.10292 mL	0.05000 mL	4.800	-0.01859	0.91342	0.00096	15.0 s
46:50.7	Data point 41	1.50000 mL	0.10861 mL	0.10303 mL	0.05000 mL	5.083	-0.01985	0.98349	0.00099	23.0 s
47:44.2	Data point 42	1.50000 mL	0.10861 mL	0.10313 mL	0.05000 mL	5.579	-0.01759	0.91486	0.00091	42.0 s
49:02.1	Data point 43	1.50000 mL	0.10861 mL	0.10320 mL	0.05000 mL	6.101	-0.01900	0.90215	0.00099	54.5 s
50:27.2	Data point 44	1.50000 mL	0.10861 mL	0.10327 mL	0.05000 mL	6.674	-0.03446	0.99241	0.00171	Timed out at 59.5 s
51:57.7	Data point 45	1.50000 mL	0.10861 mL	0.10336 mL	0.05000 mL	7.259	-0.06329	0.99069	0.00314	Timed out at 59.5 s
53:33.3	Data point 46	1.50000 mL	0.10861 mL	0.10343 mL	0.05000 mL	7.768	-0.05820	0.98124	0.00290	Timed out at 59.5 s
55:03.8	Data point 47	1.50000 mL	0.10861 mL	0.10348 mL	0.05000 mL	8.292	-0.03946	0.97572	0.00197	Timed out at 59.5 s
56:34.3	Data point 48	1.50000 mL	0.10861 mL	0.10353 mL	0.05000 mL	8.557	-0.01940	0.93969	0.00099	57.5 s
58:07.5	Data point 49	1.50000 mL	0.10861 mL	0.10360 mL	0.05000 mL	8.805	-0.00522	0.06822	0.00099	30.5 s
59:13.7	Data point 50	1.50000 mL	0.10861 mL	0.10369 mL	0.05000 mL	9.024	-0.01835	0.91843	0.00094	25.0 s
1:00:42.8	Data point 51	1.50000 mL	0.16823 mL	0.10369 mL	0.30000 mL	1.978	-0.00289	0.10876	0.00043	10.0 s
1:01:29.1	Data point 52	1.50000 mL	0.16823 mL	0.12458 mL	0.30000 mL	2.182	-0.01606	0.64737	0.00099	15.5 s
1:02:10.3	Data point 53	1.50000 mL	0.16823 mL	0.13763 mL	0.30000 mL	2.373	0.00806	0.16357	0.00099	13.0 s
1:02:49.0	Data point 54	1.50000 mL	0.16823 mL	0.14661 mL	0.30000 mL	2.587	-0.00022	0.00759	0.00012	10.0 s
1:03:24.5	Data point 55	1.50000 mL	0.16823 mL	0.15263 mL	0.30000 mL	2.790	-0.00959	0.75034	0.00055	10.0 s
1:04:00.1	Data point 56	1.50000 mL	0.16823 mL	0.15675 mL	0.30000 mL	3.013	0.01134	0.31455	0.00100	11.5 s
1:04:37.1	Data point 57	1.50000 mL	0.16823 mL	0.15941 mL	0.30000 mL	3.278	-0.01412	0.56497	0.00093	10.0 s
1:05:27.9	Data point 58	1.50000 mL	0.16823 mL	0.16087 mL	0.30000 mL	3.486	0.00232	0.15736	0.00029	10.5 s
1:06:03.8	Data point 59	1.50000 mL	0.16823 mL	0.16185 mL	0.30000 mL	3.728	-0.00733	0.87321	0.00039	10.0 s
1:06:44.4	Data point 60	1.50000 mL	0.16823 mL	0.16254 mL	0.30000 mL	3.996	-0.01008	0.94298	0.00051	10.5 s
1:07:25.5	Data point 61	1.50000 mL	0.16823 mL	0.16289 mL	0.30000 mL	4.206	-0.01231	0.75314	0.00070	10.0 s
1:08:00.9	Data point 62	1.50000 mL	0.16823 mL	0.16308 mL	0.30000 mL	4.435	0.00196	0.01015	0.00096	13.5 s
1:08:39.8	Data point 63	1.50000 mL	0.16823 mL	0.16319 mL	0.30000 mL	4.623	-0.01066	0.39352	0.00084	12.0 s
1:09:22.3	Data point 64	1.50000 mL	0.16823 mL	0.16331 mL	0.30000 mL	4.896	-0.01695	0.88825	0.00089	13.5 s
1:10:06.3	Data point 65	1.50000 mL	0.16823 mL	0.16345 mL	0.30000 mL	5.367	-0.01896	0.91841	0.00098	47.5 s
1:11:24.4	Data point 66	1.50000 mL	0.16823 mL	0.16352 mL	0.30000 mL	5.813	0.00169	0.01098	0.00080	43.0 s
1:12:38.1	Data point 67	1.50000 mL	0.16823 mL	0.16357 mL	0.30000 mL	6.350	-0.02811	0.94564	0.00143	Timed out at 59.5 s
1:14:03.5	Data point 68	1.50000 mL	0.16823 mL	0.16362 mL	0.30000 mL	6.671	-0.04606	0.97751	0.00230	Timed out at 59.5 s
1:15:39.1	Data point 69	1.50000 mL	0.16823 mL	0.16369 mL	0.30000 mL	7.163	-0.06931	0.98791	0.00344	Timed out at 59.5 s
1:17:09.6	Data point 70	1.50000 mL	0.16823 mL	0.16376 mL	0.30000 mL	7.616	-0.08650	0.98058	0.00432	Timed out at 59.5 s
1:18:40.1	Data point 71	1.50000 mL	0.16823 mL	0.16381 mL	0.30000 mL	8.042	-0.06118	0.94917	0.00310	Timed out at 59.5 s
1:20:15.7	Data point 72	1.50000 mL	0.16823 mL	0.16388 mL	0.30000 mL	8.385	-0.04572	0.94304	0.00233	Timed out at 59.5 s
1:21:51.3	Data point 73	1.50000 mL	0.16823 mL	0.16395 mL	0.30000 mL	8.716	-0.01968	0.98797	0.00098	33.5 s
1:23:05.7	Data point 74	1.50000 mL	0.16823 mL	0.16406 mL	0.30000 mL	8.959	-0.01414	0.95962	0.00071	24.5 s
1:23:55.6	Data point 75	1.50000 mL	0.16823 mL	0.16409 mL	0.30000 mL	9.002	-0.01249	0.43204	0.00094	13.5 s
1:24:18.2	Assay volumes	1.50000 mL	0.16823 mL	0.16409 mL	0.30000 mL					

Sample name: **M02_octanol**   Experiment start time: **3/3/2018 3:08:32 PM**
Assay name: **pH-metric high logP**   Analyst: **Dorothy Levorse**
Assay ID: **18C-03012**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Dorothy Levorse			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	9.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.020 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	120 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.030 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.250 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.111	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus S	0.9988	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jH	1.0	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jOH	-0.8	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r
Base concentration factor	1.000	3/3/2018 3:08:32 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.999	3/3/2018 3:08:32 PM	C:\Sirius_T3\HCl18C02.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+6.14 mV		3/3/2018 3:09:00 PM
Filling solution	3M KCl	KCL097	3/2/2018 9:43:24 AM
Liquids			
Wash 1	50% IPA:50% Water		3/2/2018 9:45:12 AM
Wash 2	0.5% Trition X-100 in H20		3/2/2018 9:45:15 AM
Buffer position 1	pH7 Wash		3/2/2018 9:45:18 AM
Buffer position 2	pH 7		3/2/2018 9:45:21 AM
Storage position			3/2/2018 9:44:44 AM
Wash water	6.7e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	8.8e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	120:41:49		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:37] Air gap created for Water (0.15 M KCl)
[2:38] Air gap created for Acid (0.5 M HCl)
[2:38] Air gap created for Base (0.5 M KOH)
[2:39] Air gap released for Water (0.15 M KCl)
[2:42] Titrator arm moved over Titration position
[2:42] Titration 1 of 3
[2:42] Adding initial titrants
[2:42] Automatically add 1.50000 mL of water
[3:08] Dispensed 1.500000 mL of Water (0.15 M KCl)
[3:12] Titrator arm moved over Drain
[5:53] Titrator arm moved to Titration position
[5:53] Argon flow rate set to 100
[5:53] Stirrer speed set to 10
[5:58] Automatically add 0.02000 mL of Octanol
[5:59] Dispensed 0.019991 mL of Octanol
[6:00] Initial pH = 9.32
[6:00] Iterative adjust 9.32 -> 2.00
[6:00] pH 9.32 -> 2.00
[6:02] Air gap released for Acid (0.5 M HCl)
[6:02] Dispensed 0.053363 mL of Acid (0.5 M HCl)
[6:08] Holding pH 2.00
[8:08] Stirrer speed set to 0
[8:08] Stirrer speed set to 50
[8:08] Iterative adjust 1.99 -> 2.00
[8:08] pH 1.99 -> 2.00
[8:08] Air gap released for Base (0.5 M KOH)
[8:09] Dispensed 0.001129 mL of Base (0.5 M KOH)
[8:59] Stirrer speed set to 0
[9:09] Datapoint id 1 collected
[9:09] Stirrer speed set to 50
[9:15] pH 2.08 -> 2.28
[9:15] Using cautious pH adjust
[9:15] Dispensed 0.006726 mL of Base (0.5 M KOH)
[9:20] Stepping pH = 2.16
[9:20] Dispensed 0.005738 mL of Base (0.5 M KOH)
[9:25] Stepping pH = 2.25
[9:25] Dispensed 0.001834 mL of Base (0.5 M KOH)
[9:31] Stepping pH = 2.28
[9:46] Stirrer speed set to 0
[9:56] Datapoint id 2 collected
[9:56] Charge balance equation is out by -6.2%
[9:56] Stirrer speed set to 50

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[10:01] pH 2.29 -> 2.49
[10:01] Using charge balance adjust
[10:01] Dispensed 0.008866 mL of Base (0.5 M KOH)
[10:21] Stirrer speed set to 0
[10:32] Datapoint id 3 collected
[10:32] Charge balance equation is out by -5.7%
[10:32] Stirrer speed set to 50
[10:37] pH 2.48 -> 2.68
[10:37] Using charge balance adjust
[10:37] Dispensed 0.006279 mL of Base (0.5 M KOH)
[10:57] Stirrer speed set to 0
[11:07] Datapoint id 4 collected
[11:07] Charge balance equation is out by -6.6%
[11:07] Stirrer speed set to 50
[11:13] pH 2.68 -> 2.88
[11:13] Using charge balance adjust
[11:13] Dispensed 0.004704 mL of Base (0.5 M KOH)
[11:33] Stirrer speed set to 0
[11:43] Datapoint id 5 collected
[11:43] Charge balance equation is out by -0.6%
[11:43] Stirrer speed set to 50
[11:48] pH 2.88 -> 3.08
[11:48] Using charge balance adjust
[11:48] Dispensed 0.003622 mL of Base (0.5 M KOH)
[12:08] Stirrer speed set to 0
[12:18] Datapoint id 6 collected
[12:18] Charge balance equation is out by 0.1%
[12:18] Stirrer speed set to 50
[12:24] pH 3.09 -> 3.29
[12:24] Using charge balance adjust
[12:24] Dispensed 0.002846 mL of Base (0.5 M KOH)
[12:44] Stirrer speed set to 0
[12:54] Datapoint id 7 collected
[12:54] Charge balance equation is out by -4.2%
[12:54] Stirrer speed set to 50
[12:59] pH 3.28 -> 3.48
[12:59] Using charge balance adjust
[13:01] Dispensed 0.002211 mL of Base (0.5 M KOH)
[13:20] Stirrer speed set to 0
[13:31] Datapoint id 8 collected
[13:31] Charge balance equation is out by 21.6%
[13:31] Stirrer speed set to 50
[13:36] pH 3.53 -> 3.73
[13:36] Using cautious pH adjust
[13:36] Dispensed 0.000776 mL of Base (0.5 M KOH)
[13:41] Stepping pH = 3.67
[13:41] Dispensed 0.000282 mL of Base (0.5 M KOH)
[13:46] Stepping pH = 3.70
[13:46] Dispensed 0.000188 mL of Base (0.5 M KOH)
[13:51] Stepping pH = 3.72
[14:07] Stirrer speed set to 0
[14:18] Datapoint id 9 collected
[14:18] Charge balance equation is out by 19.9%
[14:18] Stirrer speed set to 50
[14:23] pH 3.69 -> 3.89
[14:23] Using cautious pH adjust
[14:23] Dispensed 0.000588 mL of Base (0.5 M KOH)
[14:28] Stepping pH = 3.82
[14:29] Dispensed 0.000235 mL of Base (0.5 M KOH)

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[14:34] Stepping pH = 3.86
[14:34] Dispensed 0.000141 mL of Base (0.5 M KOH)
[14:39] Stepping pH = 3.88
[14:54] Stirrer speed set to 0
[15:08] Datapoint id 10 collected
[15:08] Charge balance equation is out by 17.0%
[15:08] Stirrer speed set to 50
[15:14] pH 3.87 -> 4.07
[15:14] Using cautious pH adjust
[15:14] Dispensed 0.000423 mL of Base (0.5 M KOH)
[15:19] Stepping pH = 4.00
[15:19] Dispensed 0.000165 mL of Base (0.5 M KOH)
[15:24] Stepping pH = 4.02
[15:24] Dispensed 0.000212 mL of Base (0.5 M KOH)
[15:29] Stepping pH = 4.09
[15:44] Stirrer speed set to 0
[16:00] Datapoint id 11 collected
[16:00] Charge balance equation is out by 4.0%
[16:00] Stirrer speed set to 50
[16:05] pH 4.05 -> 4.25
[16:05] Using charge balance adjust
[16:05] Dispensed 0.000588 mL of Base (0.5 M KOH)
[16:25] Stirrer speed set to 0
[16:53] Datapoint id 12 collected
[16:53] Charge balance equation is out by -3.7%
[16:53] Stirrer speed set to 50
[16:58] pH 4.27 -> 4.47
[16:58] Using charge balance adjust
[16:58] Dispensed 0.000376 mL of Base (0.5 M KOH)
[17:19] Stirrer speed set to 0
[17:55] Datapoint id 13 collected
[17:55] Charge balance equation is out by -71.4%
[17:55] Stirrer speed set to 50
[18:00] pH 4.37 -> 4.57
[18:00] Using cautious pH adjust
[18:00] Dispensed 0.000141 mL of Base (0.5 M KOH)
[18:05] Stepping pH = 4.42
[18:05] Dispensed 0.000212 mL of Base (0.5 M KOH)
[18:11] Stepping pH = 4.67
[18:26] Stirrer speed set to 0
[19:21] Datapoint id 14 collected
[19:21] Charge balance equation is out by -17.2%
[19:21] Stirrer speed set to 50
[19:26] pH 4.58 -> 4.78
[19:26] Using cautious pH adjust
[19:26] Dispensed 0.000094 mL of Base (0.5 M KOH)
[19:31] Stepping pH = 4.63
[19:31] Dispensed 0.000141 mL of Base (0.5 M KOH)
[19:36] Stepping pH = 4.85
[19:51] Stirrer speed set to 0
[20:51] Datapoint id 15 collected
[20:51] Charge balance equation is out by -20.7%
[20:51] Stirrer speed set to 50
[20:56] pH 4.78 -> 4.98
[20:56] Using cautious pH adjust
[20:56] Dispensed 0.000071 mL of Base (0.5 M KOH)
[21:01] Stepping pH = 4.82
[21:01] Dispensed 0.000118 mL of Base (0.5 M KOH)
[21:07] Stepping pH = 5.08

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[21:22] Stirrer speed set to 0
[22:22] Datapoint id 16 collected
[22:22] Charge balance equation is out by -35.6%
[22:22] Stirrer speed set to 50
[22:27] pH 5.00 -> 5.20
[22:27] Using cautious pH adjust
[22:27] Dispensed 0.000047 mL of Base (0.5 M KOH)
[22:32] Stepping pH = 5.11
[22:32] Dispensed 0.000024 mL of Base (0.5 M KOH)
[22:37] Stepping pH = 5.09
[22:37] Dispensed 0.000141 mL of Base (0.5 M KOH)
[22:42] Stepping pH = 5.51
[22:57] Stirrer speed set to 0
[23:53] Datapoint id 17 collected
[23:53] Charge balance equation is out by -140.4%
[23:53] Stirrer speed set to 50
[23:59] pH 5.46 -> 5.66
[23:59] Using cautious pH adjust
[23:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[24:04] Stepping pH = 5.45
[24:04] Dispensed 0.000118 mL of Base (0.5 M KOH)
[24:09] Stepping pH = 5.76
[24:24] Stirrer speed set to 0
[25:11] Datapoint id 18 collected
[25:11] Charge balance equation is out by -211.0%
[25:11] Stirrer speed set to 50
[25:16] pH 5.83 -> 6.03
[25:16] Using cautious pH adjust
[25:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[25:21] Stepping pH = 5.82
[25:21] Dispensed 0.000118 mL of Base (0.5 M KOH)
[25:26] Stepping pH = 6.32
[25:41] Stirrer speed set to 0
[26:41] Datapoint id 19 collected
[26:41] Charge balance equation is out by -217.8%
[26:41] Stirrer speed set to 50
[26:46] pH 6.25 -> 6.45
[26:46] Using cautious pH adjust
[26:46] Dispensed 0.000024 mL of Base (0.5 M KOH)
[26:51] Stepping pH = 6.23
[26:51] Dispensed 0.000118 mL of Base (0.5 M KOH)
[26:57] Stepping pH = 7.03
[27:12] Stirrer speed set to 0
[28:12] Datapoint id 20 collected
[28:12] Charge balance equation is out by -227.6%
[28:12] Stirrer speed set to 50
[28:17] pH 7.10 -> 7.30
[28:17] Using cautious pH adjust
[28:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[28:22] Stepping pH = 7.16
[28:22] Dispensed 0.000024 mL of Base (0.5 M KOH)
[28:27] Stepping pH = 7.53
[28:42] Stirrer speed set to 0
[29:42] Datapoint id 21 collected
[29:42] Charge balance equation is out by -180.3%
[29:42] Stirrer speed set to 50
[29:47] pH 7.45 -> 7.65
[29:47] Using cautious pH adjust
[29:47] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M02_octanol**   Experiment start time: **3/3/2018 3:08:32 PM**
Assay name: **pH-metric high logP**   Analyst: **Dorothy Levorse**
Assay ID: **18C-03012**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[29:52] Stepping pH = 7.65
[30:07] Stirrer speed set to 0
[31:08] Datapoint id 22 collected
[31:08] Charge balance equation is out by -150.3%
[31:08] Stirrer speed set to 50
[31:13] pH 7.60 -> 7.80
[31:13] Using cautious pH adjust
[31:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[31:18] Stepping pH = 7.75
[31:18] Dispensed 0.000024 mL of Base (0.5 M KOH)
[31:23] Stepping pH = 8.16
[31:38] Stirrer speed set to 0
[32:38] Datapoint id 23 collected
[32:38] Charge balance equation is out by -495.8%
[32:38] Stirrer speed set to 50
[32:43] pH 8.06 -> 8.26
[32:43] Using cautious pH adjust
[32:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[32:48] Stepping pH = 8.02
[32:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[32:53] Stepping pH = 8.38
[33:08] Stirrer speed set to 0
[34:09] Datapoint id 24 collected
[34:09] Charge balance equation is out by -485.1%
[34:09] Stirrer speed set to 50
[34:14] pH 8.42 -> 8.62
[34:14] Using cautious pH adjust
[34:14] Dispensed 0.000024 mL of Base (0.5 M KOH)
[34:19] Stepping pH = 8.39
[34:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[34:24] Stepping pH = 8.57
[34:24] Dispensed 0.000024 mL of Base (0.5 M KOH)
[34:29] Stepping pH = 8.82
[34:44] Stirrer speed set to 0
[35:42] Datapoint id 25 collected
[35:42] Charge balance equation is out by -501.8%
[35:42] Stirrer speed set to 50
[35:47] pH 8.72 -> 8.92
[35:47] Using cautious pH adjust
[35:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[35:52] Stepping pH = 8.69
[35:52] Dispensed 0.000071 mL of Base (0.5 M KOH)
[35:57] Stepping pH = 9.04
[36:12] Stirrer speed set to 0
[36:48] Datapoint id 26 collected
[36:48] Charge balance equation is out by -260.2%
[36:48] Titration 2 of 3
[36:48] Adding initial titrants
[36:48] Automatically add 0.03000 mL of Octanol
[36:49] Dispensed 0.030009 mL of Octanol
[36:49] Stirrer speed set to 10
[36:50] Stirrer speed set to 55
[36:50] Iterative adjust 9.10 -> 2.00
[36:50] pH 9.10 -> 2.00
[36:51] Dispensed 0.055245 mL of Acid (0.5 M HCl)
[37:41] Stirrer speed set to 0
[37:52] Datapoint id 27 collected
[37:52] Stirrer speed set to 55
[37:57] pH 1.99 -> 2.19

Sample name: **M02_octanol**　　　　　Experiment start time: **3/3/2018 3:08:32 PM**
Assay name: **pH-metric high logP**　　　　Analyst: **Dorothy Levorse**
Assay ID: **18C-03012**　　　　　　　　Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[37:57] Using cautious pH adjust
[37:57] Dispensed 0.008913 mL of Base (0.5 M KOH)
[38:02] Stepping pH = 2.08
[38:02] Dispensed 0.006279 mL of Base (0.5 M KOH)
[38:07] Stepping pH = 2.17
[38:08] Dispensed 0.001176 mL of Base (0.5 M KOH)
[38:13] Stepping pH = 2.19
[38:28] Stirrer speed set to 0
[38:38] Datapoint id 28 collected
[38:38] Charge balance equation is out by 8.2%
[38:38] Stirrer speed set to 55
[38:43] pH 2.21 -> 2.41
[38:43] Using charge balance adjust
[38:43] Dispensed 0.011406 mL of Base (0.5 M KOH)
[39:04] Stirrer speed set to 0
[39:14] Datapoint id 29 collected
[39:14] Charge balance equation is out by -5.6%
[39:14] Stirrer speed set to 55
[39:19] pH 2.40 -> 2.60
[39:19] Using charge balance adjust
[39:19] Dispensed 0.007949 mL of Base (0.5 M KOH)
[39:39] Stirrer speed set to 0
[39:50] Datapoint id 30 collected
[39:50] Charge balance equation is out by 8.8%
[39:50] Stirrer speed set to 55
[39:55] pH 2.63 -> 2.83
[39:55] Using charge balance adjust
[39:55] Dispensed 0.005480 mL of Base (0.5 M KOH)
[40:15] Stirrer speed set to 0
[40:25] Datapoint id 31 collected
[40:25] Charge balance equation is out by -9.5%
[40:25] Stirrer speed set to 55
[40:30] pH 2.82 -> 3.02
[40:30] Using charge balance adjust
[40:31] Dispensed 0.004092 mL of Base (0.5 M KOH)
[40:51] Stirrer speed set to 0
[41:01] Datapoint id 32 collected
[41:01] Charge balance equation is out by -0.9%
[41:01] Stirrer speed set to 55
[41:06] pH 3.02 -> 3.22
[41:06] Using charge balance adjust
[41:06] Dispensed 0.002987 mL of Base (0.5 M KOH)
[41:26] Stirrer speed set to 0
[41:36] Datapoint id 33 collected
[41:36] Charge balance equation is out by -4.3%
[41:36] Stirrer speed set to 55
[41:41] pH 3.22 -> 3.42
[41:41] Using charge balance adjust
[41:42] Dispensed 0.002140 mL of Base (0.5 M KOH)
[42:02] Stirrer speed set to 0
[42:12] Datapoint id 34 collected
[42:12] Charge balance equation is out by 40.8%
[42:12] Stirrer speed set to 55
[42:17] pH 3.51 -> 3.71
[42:17] Using cautious pH adjust
[42:17] Dispensed 0.000635 mL of Base (0.5 M KOH)
[42:22] Stepping pH = 3.63
[42:22] Dispensed 0.000259 mL of Base (0.5 M KOH)
[42:27] Stepping pH = 3.69

Sample name: **M02_octanol** Experiment start time: **3/3/2018 3:08:32 PM**
Assay name: **pH-metric high logP** Analyst: **Dorothy Levorse**
Assay ID: **18C-03012** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[42:27] Dispensed 0.000047 mL of Base (0.5 M KOH)
[42:32] Stepping pH = 3.69
[42:32] Dispensed 0.000165 mL of Base (0.5 M KOH)
[42:38] Stepping pH = 3.74
[42:53] Stirrer speed set to 0
[43:03] Datapoint id 35 collected
[43:03] Charge balance equation is out by 12.2%
[43:03] Stirrer speed set to 55
[43:08] pH 3.74 -> 3.94
[43:08] Using charge balance adjust
[43:08] Dispensed 0.000800 mL of Base (0.5 M KOH)
[43:29] Stirrer speed set to 0
[43:40] Datapoint id 36 collected
[43:40] Charge balance equation is out by 38.4%
[43:40] Stirrer speed set to 55
[43:45] pH 4.03 -> 4.23
[43:45] Using cautious pH adjust
[43:45] Dispensed 0.000212 mL of Base (0.5 M KOH)
[43:50] Stepping pH = 4.11
[43:50] Dispensed 0.000188 mL of Base (0.5 M KOH)
[43:55] Stepping pH = 4.23
[44:10] Stirrer speed set to 0
[44:22] Datapoint id 37 collected
[44:22] Charge balance equation is out by 7.1%
[44:22] Stirrer speed set to 55
[44:27] pH 4.25 -> 4.45
[44:27] Using charge balance adjust
[44:27] Dispensed 0.000259 mL of Base (0.5 M KOH)
[44:48] Stirrer speed set to 0
[45:01] Datapoint id 38 collected
[45:01] Charge balance equation is out by -1.3%
[45:01] Stirrer speed set to 55
[45:06] pH 4.47 -> 4.67
[45:06] Using charge balance adjust
[45:06] Dispensed 0.000165 mL of Base (0.5 M KOH)
[45:26] Stirrer speed set to 0
[45:40] Datapoint id 39 collected
[45:40] Charge balance equation is out by -8.1%
[45:40] Stirrer speed set to 55
[45:45] pH 4.69 -> 4.89
[45:45] Using charge balance adjust
[45:45] Dispensed 0.000094 mL of Base (0.5 M KOH)
[46:05] Stirrer speed set to 0
[46:20] Datapoint id 40 collected
[46:20] Charge balance equation is out by -45.8%
[46:20] Stirrer speed set to 55
[46:25] pH 4.84 -> 5.04
[46:25] Using cautious pH adjust
[46:26] Dispensed 0.000047 mL of Base (0.5 M KOH)
[46:31] Stepping pH = 4.87
[46:31] Dispensed 0.000071 mL of Base (0.5 M KOH)
[46:36] Stepping pH = 5.07
[46:51] Stirrer speed set to 0
[47:14] Datapoint id 41 collected
[47:14] Charge balance equation is out by -57.4%
[47:14] Stirrer speed set to 55
[47:19] pH 5.15 -> 5.35
[47:19] Using cautious pH adjust
[47:19] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[47:24] Stepping pH = 5.16
[47:24] Dispensed 0.000071 mL of Base (0.5 M KOH)
[47:29] Stepping pH = 5.51
[47:44] Stirrer speed set to 0
[48:27] Datapoint id 42 collected
[48:27] Charge balance equation is out by -88.9%
[48:27] Stirrer speed set to 55
[48:32] pH 5.71 -> 5.91
[48:32] Using cautious pH adjust
[48:32] Dispensed 0.000024 mL of Base (0.5 M KOH)
[48:37] Stepping pH = 5.76
[48:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[48:42] Stepping pH = 5.83
[48:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[48:47] Stepping pH = 6.06
[49:02] Stirrer speed set to 0
[49:57] Datapoint id 43 collected
[49:57] Charge balance equation is out by -92.8%
[49:57] Stirrer speed set to 55
[50:02] pH 6.20 -> 6.40
[50:02] Using cautious pH adjust
[50:02] Dispensed 0.000024 mL of Base (0.5 M KOH)
[50:07] Stepping pH = 6.23
[50:07] Dispensed 0.000047 mL of Base (0.5 M KOH)
[50:12] Stepping pH = 6.63
[50:27] Stirrer speed set to 0
[51:27] Datapoint id 44 collected
[51:27] Charge balance equation is out by -69.3%
[51:27] Stirrer speed set to 55
[51:32] pH 6.63 -> 6.83
[51:32] Using cautious pH adjust
[51:33] Dispensed 0.000024 mL of Base (0.5 M KOH)
[51:38] Stepping pH = 6.63
[51:38] Dispensed 0.000071 mL of Base (0.5 M KOH)
[51:43] Stepping pH = 7.07
[51:58] Stirrer speed set to 0
[52:58] Datapoint id 45 collected
[52:58] Charge balance equation is out by -214.8%
[52:58] Stirrer speed set to 55
[53:03] pH 7.25 -> 7.45
[53:03] Using cautious pH adjust
[53:03] Dispensed 0.000024 mL of Base (0.5 M KOH)
[53:08] Stepping pH = 7.27
[53:08] Dispensed 0.000024 mL of Base (0.5 M KOH)
[53:13] Stepping pH = 7.40
[53:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[53:18] Stepping pH = 7.65
[53:33] Stirrer speed set to 0
[54:34] Datapoint id 46 collected
[54:34] Charge balance equation is out by -403.0%
[54:34] Stirrer speed set to 55
[54:39] pH 7.78 -> 7.98
[54:39] Using cautious pH adjust
[54:39] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:44] Stepping pH = 7.88
[54:44] Dispensed 0.000024 mL of Base (0.5 M KOH)
[54:49] Stepping pH = 8.12
[55:04] Stirrer speed set to 0
[56:04] Datapoint id 47 collected

Sample name: **M02_octanol**   Experiment start time: **3/3/2018 3:08:32 PM**
Assay name: **pH-metric high logP**   Analyst: **Dorothy Levorse**
Assay ID: **18C-03012**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[56:04] Charge balance equation is out by -511.7%
[56:04] Stirrer speed set to 55
[56:09] pH 8.34 -> 8.54
[56:09] Using cautious pH adjust
[56:09] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:14] Stepping pH = 8.38
[56:14] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:19] Stepping pH = 8.53
[56:35] Stirrer speed set to 0
[57:32] Datapoint id 48 collected
[57:32] Charge balance equation is out by -253.0%
[57:32] Stirrer speed set to 55
[57:37] pH 8.57 -> 8.77
[57:37] Using cautious pH adjust
[57:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:42] Stepping pH = 8.59
[57:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:47] Stepping pH = 8.67
[57:48] Dispensed 0.000024 mL of Base (0.5 M KOH)
[57:53] Stepping pH = 8.77
[58:08] Stirrer speed set to 0
[58:38] Datapoint id 49 collected
[58:38] Charge balance equation is out by -278.9%
[58:38] Stirrer speed set to 55
[58:43] pH 8.82 -> 9.02
[58:43] Using cautious pH adjust
[58:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[58:49] Stepping pH = 8.83
[58:49] Dispensed 0.000047 mL of Base (0.5 M KOH)
[58:54] Stepping pH = 8.96
[58:54] Dispensed 0.000024 mL of Base (0.5 M KOH)
[58:59] Stepping pH = 9.04
[59:14] Stirrer speed set to 0
[59:39] Datapoint id 50 collected
[59:39] Charge balance equation is out by -176.9%
[59:39] Titration 3 of 3
[59:39] Adding initial titrants
[59:39] Automatically add 0.25000 mL of Octanol
[59:45] Dispensed 0.250000 mL of Octanol
[59:45] Stirrer speed set to 10
[59:46] Stirrer speed set to 60
[59:46] Iterative adjust 9.02 -> 2.00
[59:46] pH 9.02 -> 2.00
[59:47] Dispensed 0.056656 mL of Acid (0.5 M HCl)
[59:53] pH 2.03 -> 2.00
[59:53] Dispensed 0.002963 mL of Acid (0.5 M HCl)
[1:00:43] Stirrer speed set to 0
[1:00:53] Datapoint id 51 collected
[1:00:53] Stirrer speed set to 60
[1:00:58] pH 1.99 -> 2.19
[1:00:58] Using cautious pH adjust
[1:00:58] Dispensed 0.009784 mL of Base (0.5 M KOH)
[1:01:04] Stepping pH = 2.06
[1:01:04] Dispensed 0.008984 mL of Base (0.5 M KOH)
[1:01:09] Stepping pH = 2.16
[1:01:09] Dispensed 0.002117 mL of Base (0.5 M KOH)
[1:01:14] Stepping pH = 2.19
[1:01:29] Stirrer speed set to 0
[1:01:45] Datapoint id 52 collected

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[1:01:45] Charge balance equation is out by -6.7%
[1:01:45] Stirrer speed set to 60
[1:01:50] pH 2.19 -> 2.39
[1:01:50] Using charge balance adjust
[1:01:50] Dispensed 0.013053 mL of Base (0.5 M KOH)
[1:02:11] Stirrer speed set to 0
[1:02:24] Datapoint id 53 collected
[1:02:24] Charge balance equation is out by -6.1%
[1:02:24] Stirrer speed set to 60
[1:02:29] pH 2.38 -> 2.58
[1:02:29] Using charge balance adjust
[1:02:29] Dispensed 0.008984 mL of Base (0.5 M KOH)
[1:02:49] Stirrer speed set to 0
[1:02:59] Datapoint id 54 collected
[1:02:59] Charge balance equation is out by 4.6%
[1:02:59] Stirrer speed set to 60
[1:03:04] pH 2.59 -> 2.79
[1:03:04] Using charge balance adjust
[1:03:05] Dispensed 0.006021 mL of Base (0.5 M KOH)
[1:03:25] Stirrer speed set to 0
[1:03:35] Datapoint id 55 collected
[1:03:35] Charge balance equation is out by -0.8%
[1:03:35] Stirrer speed set to 60
[1:03:40] pH 2.79 -> 2.99
[1:03:40] Using charge balance adjust
[1:03:40] Dispensed 0.004116 mL of Base (0.5 M KOH)
[1:04:00] Stirrer speed set to 0
[1:04:12] Datapoint id 56 collected
[1:04:12] Charge balance equation is out by 9.3%
[1:04:12] Stirrer speed set to 60
[1:04:17] pH 3.02 -> 3.22
[1:04:17] Using charge balance adjust
[1:04:17] Dispensed 0.002658 mL of Base (0.5 M KOH)
[1:04:37] Stirrer speed set to 0
[1:04:47] Datapoint id 57 collected
[1:04:47] Charge balance equation is out by 29.0%
[1:04:47] Stirrer speed set to 60
[1:04:52] pH 3.29 -> 3.49
[1:04:52] Using cautious pH adjust
[1:04:52] Dispensed 0.000776 mL of Base (0.5 M KOH)
[1:04:57] Stepping pH = 3.39
[1:04:58] Dispensed 0.000494 mL of Base (0.5 M KOH)
[1:05:03] Stepping pH = 3.47
[1:05:03] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:05:08] Stepping pH = 3.48
[1:05:08] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:05:13] Stepping pH = 3.49
[1:05:28] Stirrer speed set to 0
[1:05:39] Datapoint id 58 collected
[1:05:39] Charge balance equation is out by 4.0%
[1:05:39] Stirrer speed set to 60
[1:05:44] pH 3.50 -> 3.70
[1:05:44] Using charge balance adjust
[1:05:44] Dispensed 0.000988 mL of Base (0.5 M KOH)
[1:06:04] Stirrer speed set to 0
[1:06:14] Datapoint id 59 collected
[1:06:14] Charge balance equation is out by 16.0%
[1:06:14] Stirrer speed set to 60
[1:06:19] pH 3.74 -> 3.94

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[1:06:19] Using cautious pH adjust
[1:06:19] Dispensed 0.000282 mL of Base (0.5 M KOH)
[1:06:24] Stepping pH = 3.79
[1:06:24] Dispensed 0.000400 mL of Base (0.5 M KOH)
[1:06:29] Stepping pH = 3.99
[1:06:45] Stirrer speed set to 0
[1:06:55] Datapoint id 60 collected
[1:06:55] Charge balance equation is out by -17.6%
[1:06:55] Stirrer speed set to 60
[1:07:00] pH 4.01 -> 4.21
[1:07:00] Using cautious pH adjust
[1:07:00] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:07:05] Stepping pH = 4.07
[1:07:05] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:07:11] Stepping pH = 4.21
[1:07:26] Stirrer speed set to 0
[1:07:36] Datapoint id 61 collected
[1:07:36] Charge balance equation is out by -10.9%
[1:07:36] Stirrer speed set to 60
[1:07:41] pH 4.22 -> 4.42
[1:07:41] Using charge balance adjust
[1:07:41] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:08:01] Stirrer speed set to 0
[1:08:15] Datapoint id 62 collected
[1:08:15] Charge balance equation is out by 8.4%
[1:08:15] Stirrer speed set to 60
[1:08:20] pH 4.47 -> 4.67
[1:08:20] Using charge balance adjust
[1:08:20] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:08:40] Stirrer speed set to 0
[1:08:52] Datapoint id 63 collected
[1:08:52] Charge balance equation is out by -24.3%
[1:08:52] Stirrer speed set to 60
[1:08:57] pH 4.65 -> 4.85
[1:08:57] Using cautious pH adjust
[1:08:57] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:09:02] Stepping pH = 4.69
[1:09:02] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:09:07] Stepping pH = 4.89
[1:09:22] Stirrer speed set to 0
[1:09:36] Datapoint id 64 collected
[1:09:36] Charge balance equation is out by -31.4%
[1:09:36] Stirrer speed set to 60
[1:09:41] pH 4.94 -> 5.14
[1:09:41] Using cautious pH adjust
[1:09:41] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:09:46] Stepping pH = 4.94
[1:09:46] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:09:51] Stepping pH = 5.39
[1:10:07] Stirrer speed set to 0
[1:10:54] Datapoint id 65 collected
[1:10:54] Charge balance equation is out by -203.1%
[1:10:54] Stirrer speed set to 60
[1:10:59] pH 5.56 -> 5.76
[1:10:59] Using cautious pH adjust
[1:10:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:11:04] Stepping pH = 5.59
[1:11:04] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:11:10] Stepping pH = 5.78

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[1:11:25] Stirrer speed set to 0
[1:12:08] Datapoint id 66 collected
[1:12:08] Charge balance equation is out by -75.9%
[1:12:08] Stirrer speed set to 60
[1:12:13] pH 6.06 -> 6.26
[1:12:13] Using cautious pH adjust
[1:12:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:12:18] Stepping pH = 6.18
[1:12:18] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:12:23] Stepping pH = 6.42
[1:12:38] Stirrer speed set to 0
[1:13:38] Datapoint id 67 collected
[1:13:38] Charge balance equation is out by 2.6%
[1:13:38] Stirrer speed set to 60
[1:13:43] pH 6.36 -> 6.56
[1:13:43] Using charge balance adjust
[1:13:44] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:14:04] Stirrer speed set to 0
[1:15:04] Datapoint id 68 collected
[1:15:04] Charge balance equation is out by 56.6%
[1:15:04] Stirrer speed set to 60
[1:15:09] pH 6.79 -> 6.99
[1:15:09] Using cautious pH adjust
[1:15:09] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:15:14] Stepping pH = 6.87
[1:15:14] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:15:19] Stepping pH = 6.91
[1:15:19] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:15:24] Stepping pH = 7.04
[1:15:39] Stirrer speed set to 0
[1:16:39] Datapoint id 69 collected
[1:16:39] Charge balance equation is out by -89.8%
[1:16:39] Stirrer speed set to 60
[1:16:44] pH 7.20 -> 7.40
[1:16:44] Using cautious pH adjust
[1:16:44] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:16:50] Stepping pH = 7.19
[1:16:50] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:16:55] Stepping pH = 7.44
[1:17:10] Stirrer speed set to 0
[1:18:10] Datapoint id 70 collected
[1:18:10] Charge balance equation is out by -272.1%
[1:18:10] Stirrer speed set to 60
[1:18:15] pH 7.69 -> 7.89
[1:18:15] Using cautious pH adjust
[1:18:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:18:20] Stepping pH = 7.81
[1:18:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:18:25] Stepping pH = 8.01
[1:18:40] Stirrer speed set to 0
[1:19:40] Datapoint id 71 collected
[1:19:40] Charge balance equation is out by -351.4%
[1:19:40] Stirrer speed set to 60
[1:19:45] pH 8.10 -> 8.30
[1:19:45] Using cautious pH adjust
[1:19:45] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:19:51] Stepping pH = 8.16
[1:19:51] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:19:56] Stepping pH = 8.26

Sample name: **M02_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-03012**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-03012_M02_octanol_pH-metric high logP.t3r**

Experiment start time: **3/3/2018 3:08:32 PM**
Analyst: **Dorothy Levorse**
Instrument ID: **T312060**

Experiment Log (continued)

[1:19:56] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:20:01] Stepping pH = 8.39
[1:20:16] Stirrer speed set to 0
[1:21:16] Datapoint id 72 collected
[1:21:16] Charge balance equation is out by -565.1%
[1:21:16] Stirrer speed set to 60
[1:21:21] pH 8.46 -> 8.66
[1:21:21] Using cautious pH adjust
[1:21:21] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:21:26] Stepping pH = 8.52
[1:21:26] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:21:31] Stepping pH = 8.61
[1:21:31] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:21:36] Stepping pH = 8.71
[1:21:52] Stirrer speed set to 0
[1:22:25] Datapoint id 73 collected
[1:22:25] Charge balance equation is out by -283.1%
[1:22:25] Stirrer speed set to 60
[1:22:30] pH 8.76 -> 8.96
[1:22:30] Using cautious pH adjust
[1:22:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:22:35] Stepping pH = 8.80
[1:22:35] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:22:41] Stepping pH = 8.85
[1:22:41] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:22:46] Stepping pH = 8.91
[1:22:46] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:22:51] Stepping pH = 8.98
[1:23:06] Stirrer speed set to 0
[1:23:30] Datapoint id 74 collected
[1:23:30] Charge balance equation is out by -271.8%
[1:23:30] Stirrer speed set to 60
[1:23:36] pH 8.99 -> 9.05
[1:23:36] Using cautious pH adjust
[1:23:36] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:23:41] Stepping pH = 9.01
[1:23:56] Stirrer speed set to 0
[1:24:09] Datapoint id 75 collected
[1:24:09] Charge balance equation is out by -70.9%
[1:24:09] Argon flow rate set to 0
[1:24:13] Titrator arm moved over Titration position